Data Evaluation Record on the adsorption-desorption of BSA (3,4,4-trifluoro-but-3-ene-1-sulfonic acid) in five soils

MRID Number 48574836

Data Requirement: OECD Guideline: 106
EPA Guideline: 835.1230

EPA PC Code: 050410
DP barcode: 403340

Test material: BSA (3,4,4-trifluoro-but-3-ene-1-sulfonic acid)

Primary Reviewer: Martin LeMay**,** PMRA

Secondary Reviewers: James Lin, US EPA

EPA Signature:
Date: February 14, 2013

This study was reviewed as part of a global review. Therefore, the data evaluation was prepared in monograph form. This preface is a supplement to the attached monograph section and documents the review of the study for EFED.

Results Synopsis:
This study is classified as **supplementary,** since only one concentration of 1 mg/L was tested, instead of five as required. (Different conclusion from PMRA)

CITATION: Brands C. (2011e). Adsorption/Desorption of BSA on five soils. Makhteshim Chemical Works, Ltd. Report No.: R-28474, 20 December 2011. (MRID 48574836)

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Guideline: OECD Guideline No. 106
USEPA guideline 185.1230
Deviations: None

GLP: Fully GLP compliant (laboratory certified by Netherlands VWA Authority)

Executive Summary

The adsorption characteristics of BSA (3,4,4-trifluoro-but-3-ene-1-sulfonic acid) were studied in a batch equilibrium experiment using five soils: a silt loam [Fislis; pH 6.8, organic carbon 2.13%], a sandy loam [Sevelen; pH 7.4; organic carbon 1.61%], a loam [Hom, pH 7.2; organic carbon 2.36%], a loamy sand [Speyer 2.2, pH 5.4; organic carbon 2.16%], and a clay [Speyer 6S, pH 7.2; organic carbon 1.75%]. The adsorption coefficients were determined by equilibrating test soils with BSA at nominal concentration of 1 mg BSA/L at 20ºC in the dark at soil:solution ratio of 1:1.

The recovery of the control samples ranged from 96% to 99%. Mass balances were determined for Fislis, Sevelen and Horn soil system after the adsorption cycle and ranged from 90% to 97%. Following 48 hours of equilibration, no significant adsorption for BSA on soil was observed. No meaningful values could be calculated for Fislis silt loam. Only 7.8% of applied BSA was adsorbed to the Sevelen ssandy loam, 7.2% to the Horn loam, 17.9% to the Speyer 2.2 loamy sand and 7.3% to the Speyer 6S clay. K_{oc} values determined ranged between 3.5 and 10.5. BSA is expected to be very mobile in soil.

I. MATERIALS AND METHODS

A. Materials

1. Test Materials:	3,4,4-Trifluoro-but-3-ene-1-sulfonic acid, sodium salt
Description:	White powder
Lot/Batch:	215PAL44
Purity:	99.5%
CAS#:	
Stability of compound:	The test item was stable in the application solution during the treatment of the soil samples
2. Soil:	A summary of the physical and chemical properties of the soils is provided in **Table 1**.

Table 1: Soil Physiochemical Properties

Soil designation	soil type*	% sand	% silt	%clay	% OC	CEC (meq/ 100g)	pH
Fislis	silt loam	8.0	65.6	26.4	2.13	23	6.8
Sevelen	sandy loam	53.5	37.0	9.5	1.61	9	7.4
Horn	loam	38.7	36.2	25.1	2.36	22	7.2
Speyer 2.2	loamy sand	81.4	12.2	6.4	2.16	10	5.4
Speyer 6S	clay	21.9	36.0	42.1	1.75	22	7.2

* : USDA classification
% OC: percentage organic carbon
CEC: cationic exchange capacity

B. Study design

1. Experimental conditions

An adsorption/desorption kinetics experiment was performed to determine equilibrium time. A stock solution of 1588 mg BSA/L was prepared in Milli-Q water and was diluted in 0.01M $CaCl_2$ solution to obtain a spike solution of 10.0 mg/L. The slurries (approximately 10 g soil and 9 mL 0.01 M $CaCl_2$ solution were equilibrated at 20± 2°C in the dark for three days prior to spiking. The adsorption stage of the kinetic experiment was initiated by adding a weighted volume of approximately 1 mL of spike solution to the pre-equilibrated soil slurries. A control without soil and a blank sample of each soil were also prepared. The samples were equilibrated on a roller mixer at 20± 2°C in the dark. The slurries were centrifuged at 3, 6, 24 and 48 hours. A 1.8 mL aliquot of the supernatant was sampled for analysis. After 48 hours of equilibration, the remaining supernatant of each test system was decanted and weighted. The pH of the supernatants was measured. The remaining soil of one vessel of Fislis, Sevelen and Horn test system was stored for analysis. The desorption stage of the kinetic experiment was initiated by adding equal weight of fresh 0.01 M $CaCl_2$ to decanted soil samples and equilibrated on a roller mixer. At the desorption sampling times (3, 6, and 23 hours), the slurries were centrifuged. A 1.8 mL aliquot of supernatant was sampled for analysis. After the final desorption sampling step, the remaining supernatant of the Fislis, Sevelen and Horn soils was decanted and weighted. Mass balances were determined for Fislis, Sevelen and Horn test system.

In the first adsorption test, a stock solution of 11.32 mg BSA in 10 mL Milli-Q water was prepared (1132 mg/L). The stock solution was diluted in 0.01M $CaCl_2$ solution to obtain a spike solution of 100 mg/L. In the second adsorption test, a stock solution of 24.1 mg BSA in 25 mL Milli-Q water was prepared (964 mg/L). The stock solution was diluted in 0.01M $CaCl_2$ solution to obtain a spike solution of 10.0 mg/L. The slurries (approximately 100 g soil and 99 mL 0.01 M $CaCl_2$ solution in amber glass jars in the first adsorption test and approximately 15 g soil and 13.5 mL 0.01 M $CaCl_2$ solution in polypropylene tubes in the second test) were equilibrated overnight on a shaking device at 20 ± 2°C in the dark. After equilibration, the samples were spiked with 1 or 1.5 mL spike solution to obtain final BSA concentrations in the test solutions of 1 mg/L. A control without soil was included, as well as a blank sample of each soil (soil without

test substance).

The experiments were performed at 20 ± 2°C in the dark. After 48 hours of contact time, the aqueous phases were separated from the soils by either filtration or by centrifugation. In the first test, the slurries were poured over a paper filter (S&S 589) in a suction flask under vacuum. In the second test, the soil slurries were centrifuged for 10 minutes at 7000 rpm. After removal of the supernatant, the vials were centrifuged a second time (1 hour at 7000 rpm). The supernatants were combined. Additionally, a subsample of the supernatant was centrifuged at 15000 rpm.

2. Description of analytical procedure

The test substance concentrations in the solutions were determined by means of an LC/MS validated method. The soils were extracted with 50/50 (v/v) acetonitrile/water (20 mL) at 200 rpm for 60 minutes. The extracts were analysed by the same LC/MS method. The limit of quantification (LOQ) was assessed at 0.05 mg/l in 0.01M aqueous CaCl2 and 0.15 mg/kg in soil.

II. RESULTS AND DISCUSSION

A. Mass Balance

Mass balances were determined for one sample of Fislis, Sevelen and Horn test system after the adsorption stage of the kinetics experiment. The mass balances were in the range 90-97%. The recovery of the control samples was in the range 96-99%.

B. Findings

The results of the kinetic experiment showed that BSA did not adsorb significantly to the soils. The maximum adsorbed amount was 5% after 3 hours contact time with Speyer 2.2 soil. The pH of the supernatant after adsorption were 7.3 (Fislis soil), 7.7 (Sevelen soil) and 7.2 (Horn soil).

The Koc values were calculated from one concentration due to the low amount adsorbed. Due to the low adsorption of BSA, no Freundlich isotherms coefficients could be determined. In the first adsorption test, K_d values were ≤ 0.1 and K_{OC} values were ≤ 4.4 mL/g. The pH of the supernatants ranged from 7.6 to 8.8. In the second adsorption test, K_d ranged from 0.09 to 0.23 and K_{OC} ranged from 3.5 to 10.5 for Sevelen, Horn, Speyer 2.2 and Speyer 6S soils. No meaningful values could be determined for the Fislis soil. The pH ranged from 7.3 to 8.1. The adsorption results are presented in **Table 3**.

Table 3: Adsorption characteristics of BSA on Soil based on the final adsorption test

Soil designation	pH	% OC	Koc
Fislis	6.8	2.13	#
Sevelen	7.4	1.61	5.3
Horn	7.2	2.36	3.5
Speyer 2.2	5.4	2.16	10.5
Speyer 6S	7.2	1.75	5.0

Mean	---	---	6.1

could not be calculated
% OC: percentage organic carbon

III. CONCLUSIONS

BSA is very mobile in soil. K_{oc} values determined ranged between 3.5 and 10.5.